



## Atmosphere, temperature and pressure dependent segregation of bulk impurities in yttria-stabilized zirconia

Andersen, Thomas; Jensen, Karin Vels; Mogensen, Mogens Bjerg; Chorkendorff, Ib

*Published in:*  
Meeting abstracts

*Publication date:*  
2010

*Document Version*  
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

*Citation (APA):*  
Andersen, T., Jensen, K. V., Mogensen, M. B., & Chorkendorff, I. (2010). Atmosphere, temperature and pressure dependent segregation of bulk impurities in yttria-stabilized zirconia. In *Meeting abstracts* (pp. 1391-1391). The Electrochemical Society.

---

### General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

# Atmosphere, temperature and pressure dependent segregation of bulk impurities in yttria-stabilized zirconia

T. Andersen<sup>a</sup>, K.V. Jensen<sup>b</sup>, M. Mogensen<sup>b</sup> and I. Chorkendorff<sup>a</sup>

<sup>a</sup>*Center for Individual Nanoparticle Functionality, Department of Physics, Building 312, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark*  
<sup>b</sup>*Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Technical University of Denmark, DK-4000 Roskilde, Denmark,*

Control and characterization of extremely clean surfaces are important to gain fundamental understanding of processes on surfaces. All surfaces exposed to atmospheric conditions are covered with impurity adsorbates. These adsorbates are usually mainly water and organic molecules which lower the surface free energy of the external surface of the material. In devices operated at elevated temperatures (600 – 1100 °C), such as solid oxide fuel cells (SOFCs), segregation of bulk impurities from component materials can also be observed [1].

Bulk impurities present in yttria-stabilized zirconia (YSZ), typically used as electrolyte in SOFCs, such as silicon dioxide (silica), segregates to the anode-electrolyte interface at operating conditions of SOFCs. Impurity segregation and the formation of an impurity phase on YSZ have previously been shown to increase the polarization resistance of an anode-electrolyte SOFC model system [2].

Here we report on an in-situ ultra high vacuum (UHV) study of impurity segregation in YSZ single crystals.

YSZ single crystals were heated in an UHV chamber in the temperature range 750 – 1400 °C. Oxygen and water vapor atmospheres in the pressure range from UHV to 1 bar were introduced while the single crystals were annealed in the chamber. The single crystals were after treatment transported in-situ to an analysis chamber where X-ray photoelectron spectroscopy (XPS) measurements were performed. This setup allowed for investigation of the surface composition of YSZ without exposure to air.

All single crystals annealed in a furnace (ex-situ) at atmospheric conditions (1100 °C, 1 bar) showed the formation of a silicon monolayer on the surface as characterized by angle-resolved XPS. Annealing in UHV at a range of elevated temperatures indicated a strong atmosphere dependency of silica segregation. Experiments with both low (< 1E-5 mbar) and high (> 1 mbar) pressures of water vapor and oxygen gas supported atmosphere dependence of silica segregation in YSZ. Furthermore, the experiments with water vapor and oxygen gas also revealed a temperature and pressure dependent silica segregation mechanism in YSZ.

The above findings indicate a strong dependence on atmosphere, pressure and temperature of silicon segregation in single crystal YSZ. Knowledge of the segregation process in YSZ allows for optimized cleaning cycles with the aim of producing extremely clean YSZ for electrochemical tests.

## Acknowledgements

This work was supported financially by The Programme Commission on Sustainable Energy and Environment, The Danish Council for Strategic Research, via the Strategic Electrochemistry Research Center (SERC) ([www.serc.dk](http://www.serc.dk)), contract no. 2104-06-0011.

## References

- [1] Hughes, A., Journal of the American Ceramic Society 78 (1995), 369-378
- [2] Jensen, K.V. et al, Solid State Ionics 160 (2003) 27-37